Spherical harmonics

$$Y_{lm}(\theta,\phi)=\Theta_{lm}(\theta)\mathrm{e}^{\mathrm{i}m\phi} \qquad \widehat{\mathrm{L}}^2 Y_{lm}=l(l+1)\hbar^2\,Y_{lm} \qquad \widehat{\mathrm{L}}_z Y_{lm}=m\hbar\,Y_{lm}$$

$$\text{parity of } Y_{lm}=(-1)^l \qquad l=0,1,2,\ldots \qquad m=-l,-l+1,\ldots,l-1,l$$

$$\int_0^{2\pi}\int_0^{\pi} Y^*_{l_1,m_1}(\theta,\phi)Y_{l_2,m_2}(\theta,\phi)\,\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi=\delta_{l_1,l_2}\delta_{m_1,m_2} \qquad \int_0^{2\pi}\int_0^{\pi}|Y_{l,m}(\theta,\phi)|^2\,\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi=1$$

Hydrogen and hydrogen-like atoms

$$\widehat{\mathrm{H}}=-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{\widehat{\mathrm{L}}^2}{2\mu\,r^2}-\frac{e^2}{4\pi\varepsilon_0\,r} \qquad \widehat{\mathrm{H}}\psi_{nlm}=E_n\psi_{nlm} \qquad n=1,\,2,\,\ldots;\quad l=0,\,1,\,2\,\ldots,\,n-1$$

$$\psi_{nlm}(r,\theta,\phi)=R_{nl}(r)Y_{lm}(\theta,\phi) \qquad R_{nl}(r)=\left(\frac{r}{a_0}\right)^l\left(\text{polynomial in }\frac{r}{a_0}\right)\mathrm{e}^{-r/na_0}$$

$$\langle r^k\rangle=\int_0^\infty r^{k+2}R^2_{nl}(r)\,\mathrm{d}r \qquad \int_0^\infty R^*_{n_1,l}(r)R_{n_2,l}(r)\,r^2\,\mathrm{d}r=\delta_{n_1,n_2}$$

$$E_n=-\frac{E_\mathrm{R}}{n^2} \qquad \mu=\frac{m_1m_2}{m_1+m_2} \qquad E_\mathrm{R}=\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{\mu}{2\hbar^2}=\frac{\hbar^2}{2\mu a_0^2}=\frac{1}{2}\frac{e^2}{4\pi\varepsilon_0 a_0} \qquad a_0=\frac{4\pi\varepsilon_0}{e^2}\frac{\hbar^2}{\mu}$$

$$E_{nlj}=-\frac{E_\mathrm{R}}{n^2}\left[1+\frac{\alpha^2}{n}\left(\frac{1}{j+\frac{1}{2}}-\frac{3}{4n}\right)\right] \qquad \alpha=\frac{e^2}{4\pi\varepsilon_0\hbar c} \qquad E_\mathrm{R}^\text{scaled}=Z^2\frac{\mu}{\mu_\mathrm{H}}E_\mathrm{R} \qquad a_0^\text{scaled}=\frac{1}{Z}\frac{\mu_\mathrm{H}}{\mu}a_0$$

Spin–orbit coupling

$\mathbf{J}=\mathbf{L}+\mathbf{S}$ $\qquad$ $\widehat{\mathrm{J}}^2$ has eigenvalues $j(j+1)\hbar^2$ $\qquad$ $\widehat{\mathrm{J}}_z$ has eigenvalues $m_j\hbar$

For a spin-$\frac{1}{2}$ particle: $\qquad$ $j=l\pm\frac{1}{2}$ $\qquad$ $m_j=-j,\,-j+1,\,\ldots,\,j-1,\,j$

Terms from configuration with non-equivalent valence electrons (l_1,s_1) and (l_2,s_2):

$$L=|l_1-l_2|,\,|l_1-l_2|+1,\,\ldots,\,l_1+l_2-1,\,l_1+l_2 \qquad S=|s_1-s_2|,\,|s_1-s_2|+1,\,\ldots,\,s_1+s_2-1,\,s_1+s_2$$

LS-coupling: levels from term with L and S: $\qquad$ $J=|L-S|,\,|L-S|+1,\,\ldots,\,L+S-1,L+S$

Approximation methods

$$E_\mathrm{gs}\le\min\frac{\langle\phi_\mathrm{t}|\widehat{\mathrm{H}}|\phi_\mathrm{t}\rangle}{\langle\,\phi_\mathrm{t}|\phi_\mathrm{t}\,\rangle} \qquad \widehat{\mathrm{H}}=\widehat{\mathrm{H}}^{(0)}+\delta\widehat{\mathrm{H}} \qquad \widehat{\mathrm{H}}^{(0)}\psi_n^{(0)}=E_n^{(0)}\psi_n^{(0)} \qquad E_n\simeq E_n^{(0)}+\langle\psi_n^{(0)}|\delta\widehat{\mathrm{H}}|\psi_n^{(0)}\rangle$$

$$\Psi(x,t)=\sum_k a_k(t)\psi_k(x)\mathrm{e}^{-\mathrm{i}E_kt/\hbar} \qquad a_k(t)\simeq\delta_{ki}+\frac{1}{\mathrm{i}\hbar}\int_0^t\mathrm{e}^{\mathrm{i}\omega_{ki}t'}V_{ki}(t')\,\mathrm{d}t' \qquad l_f=l_i\pm1;\ m_f=m_i\text{ or }m_i\pm1$$

Group / Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub						

s shells filling
p shells filling
d shells filling
4f shell filling
5f shell filling

6	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
7	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

1 hydrogen; 2 helium; 3 lithium; 4 beryllium; 5 boron; 6 carbon; 7 nitrogen; 8 oxygen; 9 fluorine; 10 neon; 11 sodium; 12 magnesium; 13 aluminium; 14 silicon; 15 phosphorus; 16 sulphur; 17 chlorine; 18 argon; 19 potassium; 20 calcium; 21 scandium; 22 titanium; 23 vanadium; 24 chromium; 25 manganese; 26 iron; 27 cobalt; 28 nickel; 29 copper; 30 zinc; 31 gallium; 32 germanium; 33 arsenic; 34 selenium; 35 bromine; 36 krypton; 37 rubidium; 38 strontium; 39 yttrium; 40 zirconium; 41 niobium; 42 molybdenum; 43 technetium; 44 ruthenium; 45 rhodium; 46 palladium; 47 silver; 48 cadmium; 49 indium; 50 tin; 51 antimony; 52 tellurium; 53 iodine; 54 xenon; 55 caesium; 56 barium; 57 lanthanum; 58 cerium; 59 praseodymium; 60 neodymium; 61 promethium; 62 samarium; 63 europium; 64 gadolinium; 65 terbium; 66 dysprosium; 67 holmium; 68 erbium; 69 thulium; 70 ytterbium; 71 lutetium; 72 hafnium; 73 tantalum; 74 tungsten; 75 rhenium; 76 osmium; 77 iridium; 78 platinum; 79 gold; 80 mercury; 81 thallium; 82 lead; 83 bismuth; 84 polonium; 85 astatine; 86 radon; 87 francium; 88 radium; 89 actinium; 90 thorium; 91 protoactinium; 92 uranium; 93 neptunium; 94 plutonium; 95 americium; 96 curium; 97 berkelium; 98 californium; 99 einsteinium; 100 fermium; 101 mendelevium; 102 nobelium; 103 lawrencium; 104 rutherfordium; 105 dubnium; 106 seaborgium; 107 bohrium; 108 hassium; 109 meitnerium; 110 darmstadtium; 111 roentgenium; 112 ununbium

Physical constants

Planck's constant	h	6.63×10^{-34} J s	Planck's constant/2π	$\hbar$	1.06×10^{-34} J s
vacuum speed of light	c	3.00×10^{8} m s^{-1}	Coulomb law constant	$\frac{1}{4\pi\varepsilon_0}$	8.99×10^{9} m F^{-1}
permittivity of free space	ε_0	8.85×10^{-12} F m^{-1}	permeability of free space	μ_0	$4\pi \times 10^{-7}$ H m^{-1}
Boltzmann's constant	k	1.38×10^{-23} J K^{-1}	Avogadro's constant	N_{m}	6.02×10^{23} mol^{-1}
electron charge	$-e$	-1.60×10^{-19} C	proton charge	e	1.60×10^{-19} C
electron mass	m_{e}	9.11×10^{-31} kg	proton mass	m_{p}	1.67×10^{-27} kg
Bohr radius	a_0	5.29×10^{-11} m	atomic mass unit	u	1.66×10^{-27} kg

Complex numbers and elementary functions $(a>0,\ b>0)$

$z = x + \mathrm{i}y = r\mathrm{e}^{\mathrm{i}\theta}$ $\quad$ $z^* = x - \mathrm{i}y = r\mathrm{e}^{-\mathrm{i}\theta}$ $\quad$ $|z|^2 = zz^* = x^2 + y^2 = r^2$

$\mathrm{Re}(z) = \dfrac{z + z^*}{2}$ $\quad$ $\mathrm{Im}(z) = \dfrac{z - z^*}{2\mathrm{i}}$ $\quad$ $z^n = r^n \mathrm{e}^{\mathrm{i}n\theta}$

$\mathrm{e}^{\mathrm{i}\theta} = \cos\theta + \mathrm{i}\sin\theta$ $\quad$ $\mathrm{e}^{\pm\mathrm{i}\pi} = -1$ $\quad$ $\mathrm{e}^{\pm\mathrm{i}\pi/2} = \pm\mathrm{i}$

$\mathrm{e}^x\mathrm{e}^y = \mathrm{e}^{x+y}$ $\quad$ $\ln a + \ln b = \ln(ab)$ $\quad$ $\mathrm{e}^{\ln a} = \ln(\mathrm{e}^a) = a$

$\cos(\theta \pm \pi) = -\cos\theta$ $\quad$ $\sin(\theta \pm \pi) = -\sin\theta$ $\quad$ $\tan(\theta \pm \pi) = \tan\theta$

$\cos(\theta \pm \pi/2) = \mp\sin\theta$ $\quad$ $\sin(\theta \pm \pi/2) = \pm\cos\theta$ $\quad$ $\tan(\theta + \pi/2) = -\cot\theta$

$\cos^2\theta + \sin^2\theta = 1$ $\quad$ $\dfrac{1}{1+x} = 1 - x + x^2 - \ldots$ $\quad$ $\dfrac{1}{1-x} = 1 + x + x^2 + \ldots$

$e^x = 1 + x + \dfrac{x^2}{2!} + \dfrac{x^3}{3!} + \ldots$ $\quad$ $\cos x = 1 - \dfrac{x^2}{2!} + \dfrac{x^4}{4!} - \ldots$ $\quad$ $\sin x = x - \dfrac{x^3}{3!} + \dfrac{x^5}{5!} - \ldots$

$\cos(A \pm B) = \cos A\cos B \mp \sin A\sin B$ $\quad$ $\sin(A \pm B) = \sin A\cos B \pm \cos A\sin B$

$\cos A\cos B = \tfrac{1}{2}\big(\cos(A-B) + \cos(A+B)\big)$ $\quad$ $\sin A\sin B = \tfrac{1}{2}\big(\cos(A-B) - \cos(A+B)\big)$

Integrals (n and m positive integers)

$$\int_{-a}^{a} f(x)\,\mathrm{d}x = 0 \qquad (f(x)\ \text{odd})$$

$$\int_{-a}^{a} f(x)\,\mathrm{d}x = 2\int_{0}^{a} f(x)\,\mathrm{d}x \qquad (f(x)\ \text{even})$$

$$\int \sin^2(x)\,\mathrm{d}x = \frac{x}{2} - \frac{1}{4}\sin(2x)$$

$$\int \cos^2(x)\,\mathrm{d}x = \frac{x}{2} + \frac{1}{4}\sin(2x)$$

$$\int_0^{\pi} \sin(nx)\sin(mx)\,\mathrm{d}x = \frac{\pi}{2}\,\delta_{nm}$$

$$\int_0^{\pi} \cos(nx)\cos(mx)\,\mathrm{d}x = \frac{\pi}{2}\,\delta_{nm}$$

$$\int_{-\pi/2}^{\pi/2} \sin(nx)\sin(mx)\,\mathrm{d}x = \frac{\pi}{2}\,\delta_{nm} \qquad (m+n\ \text{even})$$

$$\int_{-\pi/2}^{\pi/2} \cos(nx)\cos(mx)\,\mathrm{d}x = \frac{\pi}{2}\,\delta_{nm} \qquad (m+n\ \text{even})$$

$$\int_0^{\pi} \sin^{2n}(x)\,\mathrm{d}x = \frac{(2n-1)\,(2n-3)\ldots 1}{2^n n!}\,\pi$$

$$\int_0^{\pi} \sin^{2n+1}(x)\,\mathrm{d}x = \frac{2^{n+1} n!}{(2n+1)\,(2n-1)\ldots 1}$$

$$\int_0^{\pi} \cos^{2n}(x)\,\mathrm{d}x = \frac{(2n-1)\,(2n-3)\ldots 1}{2^n n!}\,\pi$$

$$\int_0^{\pi} \cos^{2n+1}(x)\,\mathrm{d}x = 0$$

$$\int_0^{\infty} x^n \mathrm{e}^{-\alpha x}\,\mathrm{d}x = \frac{n!}{\alpha^{n+1}} \quad \text{for } \mathrm{Re}(\alpha) > 0$$

$$\int_{-\infty}^{\infty} \frac{\sin^2(ax)}{x^2}\,\mathrm{d}x = \pi|a| \qquad (a\ \text{real})$$

$$\int_{-\infty}^{\infty} x^{2n}\mathrm{e}^{-x^2}\,\mathrm{d}x = \frac{(2n-1)\,(2n-3)\ldots 1}{2^n}\sqrt{\pi}$$

$$\int_{-\infty}^{\infty} \mathrm{e}^{-x^2}\,\mathrm{d}x = \sqrt{\pi}$$